4GLS – the UK's Fourth Generation Light Source

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ABSTRACT

4GLS is a suite of accelerator-based light sources planned to provide state-of-the-art radiation in the low energy photon regime. Superconducting energy recovery linac (ERL) technology will be utilised in combination with a variety of free electron lasers (IR to XUV), undulators and bending magnets. The 4GLS undulators will generate spontaneous high flux, high brightness radiation, of variable polarisation from 3 - 800 eV, optimised in the lower harmonics up to about 200 eV. Viable radiation at energies up to several keV may be provided from multipole wiggler magnet radiation. The ERL technology of 4GLS will allow shorter bunches and higher peak photon fluxes than possible from storage ring sources. It will also give users the added bonuses of pulse structure flexibility and effectively an infinite beam lifetime. VUV and XUV FELs will be used to generate short pulses (in the fs regime) of extreme ultraviolet light that is broadly tuneable and more than a million times more intense than the equivalent spontaneous undulator radiation. A strong feature of the scientific programme planned for 4GLS is dynamics experiments in a wide range of fields. Pump probe experiments will allow the study of chemical reactions and short-lived intermediates on the timescale of bond breaking and bond making, even for very dilute species. The high intensity of the FEL radiation will allow very high resolution in imaging applications. Funding for the first three years of the 4GLS project was announced by the UK Government in April 2003. This includes the research and development work necessary to produce a design study report, with the construction of an ERL-prototype. Additional funds have recently been awarded that will enable a study of the production of ultra-short pulsed X-rays from the ERL-prototype via Thomson scattering. It is anticipated that the full 4GLS facility will be available to users in 2011.

Keywords: 4th Generation Light Source, Free Electron Laser (FEL), Energy Recovery Linac (ERL)

1. THE PROPOSED 4GLS FACILITY

1.1 Introduction

In current 'third generation' synchrotron sources radiation is extracted from insertion devices ('undulators' and 'multipole wigglers'), and from the bending magnets that ensure the circulation of electrons in storage rings. The electrons circulating in such rings typically orbit the ring around 10^{11} times, and the resultant equilibration of the electron beam with its surroundings results in fundamental limitations in source brightness and pulse length. In recent years, the Energy Recovery Linac (ERL) concept[1-3] has been applied for the first time to the production of SR in two projects at the Jefferson Laboratory in Virginia. In an ERL device, a high density electron beam is produced by an RF superconducting linac array. This circulates the ring once (or only a few times), with its phase arranged so that when it returns to the linac structure, it is decelerated, returning its energy to the RF field. The Jefferson team has already demonstrated recovery of in excess of 99.98% of the beam energy[4]. In parallel with these developments has been a related programme to demonstrate the potential of free electron lasers (FELs). Such sources extend the interaction between the electrons and the undulators into a regime where huge brightness increases can be obtained. So far a number of infrared user facilities, based on low energy electron linacs, have been established (*e.g.* FELIX[5] in the

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Netherlands, the Jefferson Laboratory[4], a number of university facilities in the USA, and CLIO in France) and there have also been a limited number of successful attempts to transfer the technology onto storage rings at higher electron energy and thus produce radiation into the VUV (Super-ACO (France), ELETTRA (Italy)[6], Duke University (USA), and NIJI-IV (Japan)). These FELs, like their laser counterparts are dependent on mirrors to trap the emitted radiation in optical cavities. The SASE (self amplification of spontaneous emission) FEL, first developed at the University of California, Los Angeles, and also implemented at the DESY laboratory, is free of the constraint of mirrors and therefore has the potential for further extending output wavelengths from the XUV into the x-ray region[7,8]. The properties of high intensity, extended wavelength range, and 'laser-like' beams produced by FELs make them the sources of choice when conventional lasers or SR fail to meet the peak flux or brightness criteria for an experiment.

1.1 The 4GLS Concept

The 4GLS proposal is to site an IR-FEL, VUV-FEL, and single-pass XUV-FEL at one experimental facility, which will also provide for undulator and bending magnet radiation (Figure 1).

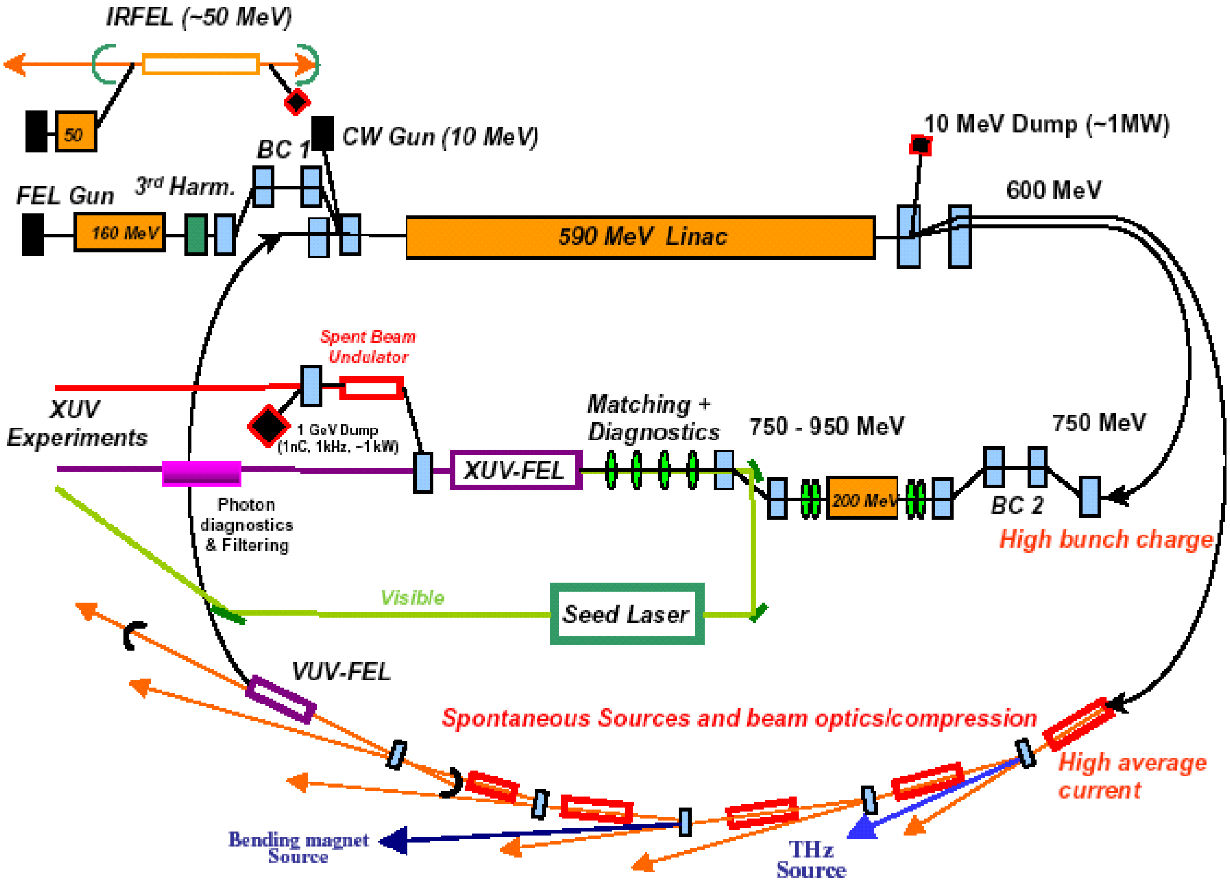

Figure 1: The conceptual layout of 4GLS

At the heart of the facility is a photocathode injected energy recovery linac (ERL) and a single pass electron return path, which allows the energy from the returning electron beam to be recovered in the ERL. The arrangement of ERL, bending magnets, undulators and FELs is designed to provide both single and bespoke combinations of sources at a multi-user facility. The machine configuration gives the advantage of a constant beam current and may be operated in either in high current (effectively CW) mode or in a ‘temporal’ mode offering a tailored train of sub-picosecond pulses.

The frequency coverage provided by the 4GLS FELs (IR-THz, VUV and XUV) is designed to complement available table-top laser sources; it is envisaged that 4GLS may be powerfully combined with these sources in many experiments.

1.3 4GLS Photon Sources

The 4GLS photon sources are described below. Their peak brightness is compared with other laser and SR sources in Figure 2.

1.3.1 The 4GLS Undulators and Bending Magnet Sources

The 4GLS undulators will be optimized to generate spontaneous high flux, high brightness radiation, of variable polarization, over the photon energy range 3 – 200 eV. However, they will also generate very intense radiation (in the higher harmonics) at energies up to about 800 eV. Typical undulators will generate fluxes of 10^{15} photons/(s.0.1%bp.100mA) and peak brightnesses up to 10^{22} photons/(s.0.1%bp.100mA.mm^2.mrad^2). The option of including a multipole wiggler magnet source, extending the useful output to *ca.* 3 keV, is being explored; an example of the output of a 2T multipole wiggler source on 4GLS is shown in Figure 2. Bending magnets on 4GLS will provide photons from the THz regime to over 1 keV. Due to the small physical size of the ring, it will be straightforward to obtain large vertical and horizontal apertures (tens of mrad). This will be of particular advantage to users who need high intensity continuous flux. The bending magnet sources will also produce coherent radiation in the IR and THz, and because the electron bunch lengths on 4GLS will be of the order of the wavelength of the emitted light for energies below 0.02 eV (160 cm^{-1}), considerable flux enhancement due to multi-particle coherent emission will occur. This enhancement has recently been demonstrated at Jefferson Laboratory[9]. In the case of 4GLS peak brightness of up to 10^{21} photons/(s.0.1%bp.100mA.mm^2.mrad^2) in the far-IR is anticipated.

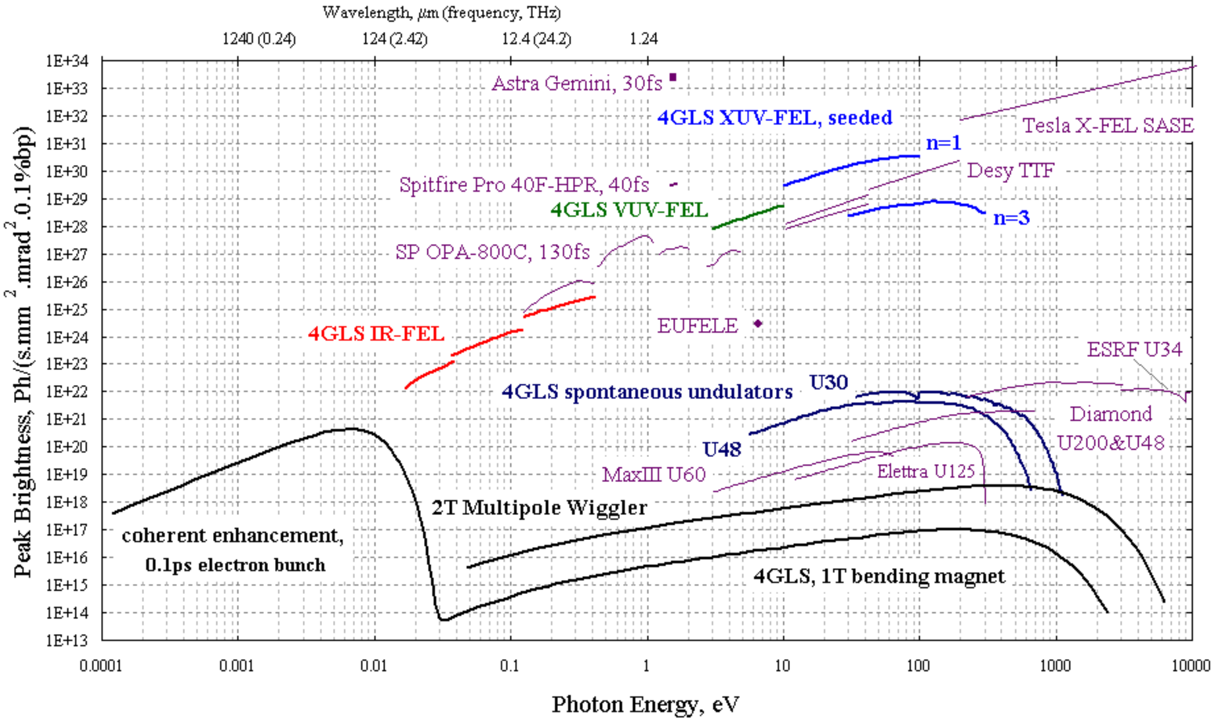

Figure 2: The peak brightness of the 4GLS sources compared with other world sources. The latter include IR and visible laser sources (such as Astra Gemini, Spitfire Pro), FELs (such as EUFELE and TESLA XFEL) and synchrotron sources including ESRF, MAXIII, ELETTRA and Diamond. In the case of the 4GLS XUV FEL, output from both the first harmonic (n=1) and third harmonic (n=3) are shown.

1.3.2 The IR-FEL

The IR-FEL will generate sub-picosecond laser pulses of variable polarisation in the range 3 to 75 μm (0.4 – 0.017 eV). The proposed design will generate very high pulse energies of between 6 and 60 μJ depending upon the output wavelength, corresponding to average fluxes of typically 10^{21} photons/s/0.1% bp. The use of superconducting RF linac technology allows for a truly continuous output at the design repetition rate of 13 MHz, rather than operating in macropulse 'burst' mode common to almost all other IR-FEL user facilities. The 4GLS IR-FEL will be based on a multi-pass optical cavity and its output will be diffraction and transform limited over its operating range. It will have the facility to operate either independently or synchronously with the other 4GLS sources shown in Figure 1.

1.3.3 The VUV-FEL

The proposed VUV-FEL is based on an optical cavity arrangement. Such systems have been successfully implemented in several storage ring facilities. The success of existing storage ring FELs has depended heavily on the development of very high reflectivity multilayer mirrors, with reflectivities of 95% or better[10], and this has limited the short wavelength performance of current devices to around 170 nm. However, it is expected that, by the use of pure Al mirrors, the limit will be extended to 120 nm in the near future[11]. The cavity concept that has been developed for 4GLS has high gain due to the extremely high quality electron beam and does not rely on very high reflectivity mirrors; simulations suggest that reflectivities of the order of 50% will be adequate, giving plenty of design margin. However, an alternative design based on a seeded single pass amplifier, which would eliminate the need for high reflectivity mirrors, could be considered for this FEL should this relaxed mirror specification prove to be too demanding. The cavity based VUV-FEL will produce an average photon flux ouput of around 10^{21} photons/s, a peak flux of about 10^{26} photons/s (10^{14} photons/pulse) at a repetition rate of 6.5 MHz (with a pulse energy of *ca.* 100 μJ). The FEL will be designed to produce variably polarised, sub-picosecond VUV pulses that will be broadly tunable in the range from the visible to 10 eV. The output of the VUV-FEL will be 10 orders of magnitude more intense in terms of peak brightness than the spontaneous VUV radiation from undulators on third generation sources.

1.3.4. The XUV-FEL

Without the constraints of a cavity and its associated mirrors the XUV-FEL on 4GLS is designed to generate variable polarisation photons well into the extreme ultraviolet and even the soft x-ray region. Intense, short duration electron bunches fed into the long undulator lead to exponential growth of the photon peak power giving highly intense and coherent radiation. These high gain amplifier FELs require long, high-precision undulators for their operation. The present design is 'seeded' by an HHG laser source over the 10 to 100 eV range by feeding the HHG produced light into the entrance of the undulator, overlapping with the electron bunch. This seed forces the electron beam to lase at the required photon energy with high quality temporal, spatial and spectral pulse properties. If no seed is used (the so-called SASE regime) then the shot to shot reproducibility of the photon pulses is compromised. The XUV-FEL is presently assumed to produce single photon pulses at a repetition rate of 1 kHz with average photon fluxes in the region of 10^{17} photons/s, pulse energies in the range 150 to 400 μJ, peak fluxes of around 10^{27} photons/s and peak brightnesses in excess of 10^{30} photons/(s.0.1%bp.mm^2.mrad^2). Time-dependent simulations of the XUV FEL output using the 3D code GENESIS 1.3 are underway. Initial results indicate a FWHM photon pulse length of 100 fs is achieved in the energy range 10 – 100 eV at distances of 5 – 25 m along the undulator.

2. CURRENT STATUS OF THE 4GLS PROJECT

The project is currently subject to assessment under the Office of Government Commerce 'Gateway' Process. The science case for 4GLS[12] ('Gateway 0') was approved in April 2002. The business case ('Gateway 1') was approved in November 2002. Funding for the first three years of the 4GLS project was announced by the UK Government in April 2003. This includes the research and development work necessary to produce a design study report, with the construction of an ERL-prototype (ERLP). It is anticipated that, subject to successful passage through the remaining gateways, the full facility will be available to EU users in 2011.

3. THE 4GLS PROTOTYPE, ERLP

The 4GLS prototype is currently under construction at CCLRC Daresbury Laboratory, and it is anticipated that construction will be complete in summer 2006. The layout of the machine is shown in Figure 3. It will be used to study issues such as compression, synchronization, energy recovery and coherent synchrotron emission (CSR), in order to validate choices for 4GLS. ERLP will consist of a single-pass superconducting linac driving an oscillator FEL, circulating 80 pC electron bunches at up to 35 MeV; deceleration through the same linac 180 degrees out of phase with acceleration will provide energy recovery, with injection and extraction occurring at nominally 8.35 MeV. The injector consists of a high-average current DC photocathode gun, a booster and a transfer line to the main linac[13]. The DC photocathode gun is a replica of the 500 kV Jefferson Laboratory gun[14] and will operate at a nominal accelerating voltage of 350 kV. Electrons will be generated at a GaAs photocathode by frequency doubled light (532 nm) from a mode-locked Nd:YVO_4 laser with an oscillator frequency of 81.25 MHz. Following focusing and bunch shortening, the electrons will be accelerated to 8.35 MeV in the booster. This consists of two superconducting 9-cell TESLA-type cavities operated at 1.3 GHz. The cryomodule design is based on the design of the ELBE linac[15]. The booster is followed by a transfer line which transports the beam to the straight of the main linac where it is merged with the full energy (35 MeV) single-pass recirculated beam. The superconducting main linac is identical to the booster (two 9-cell TESLA-type cavities). Two 180 ° triple-bend achromat (TBA) arcs[16] are used to recirculate the beam to the main linac where the electrons are decelerated to their injection energy. The electrons are separated from the full energy beam by an extraction chicane and then dumped in the beam dump. A 4-dipole chicane provides bunch compression upstream of the wiggler and bypasses one of the FEL mirrors.

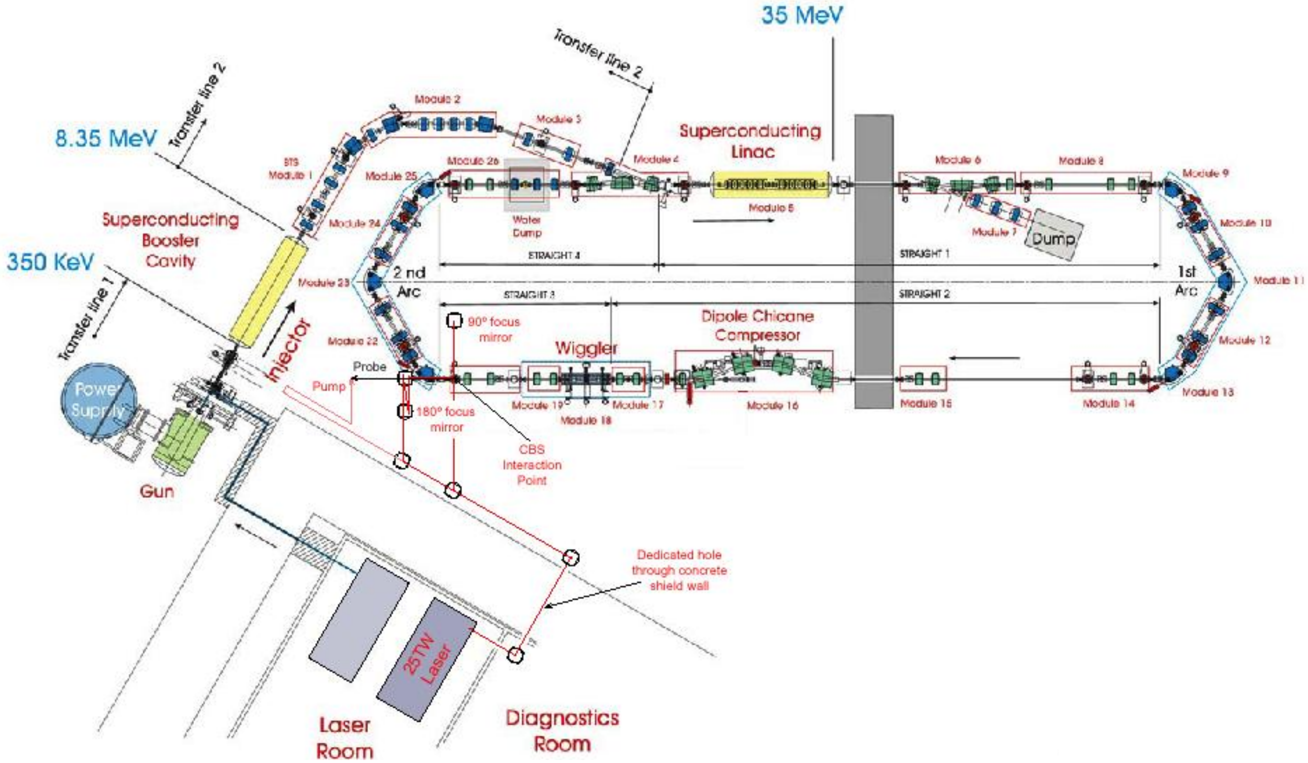

Figure 3: The layout of the 4GLS energy recovery prototype, ERLP.

The wiggler providing the IR FEL has been supplied on loan from Jefferson Laboratory, and is a planar device with 40 periods of length 27 mm. The FEL will lase at 4.3 μm, with a peak brightness of 10^{26} photons/(s.0.1%bp.100mA.mm^2.$mrad^2$). The calculated output characteristics of the IR FEL and the SR from the chicane dipole magnets are shown in Figure 4. This clearly illustrates the enhancement due to CSR emission at long wavelengths. In addition to tests of beam dynamics, a study of the production of short-pulsed X-rays by Thomson scattering will be carried out by interaction of the electron beam of ERLP with the pulse train from a 25 TW laser (800 nm 40 fs Ti:sapphire, indicated schematically in Figure 3). THz bending magnet radiation will also be used in combination with a lower power 30 fs Ti:sapphire laser system in pump-probe demonstration experiments.

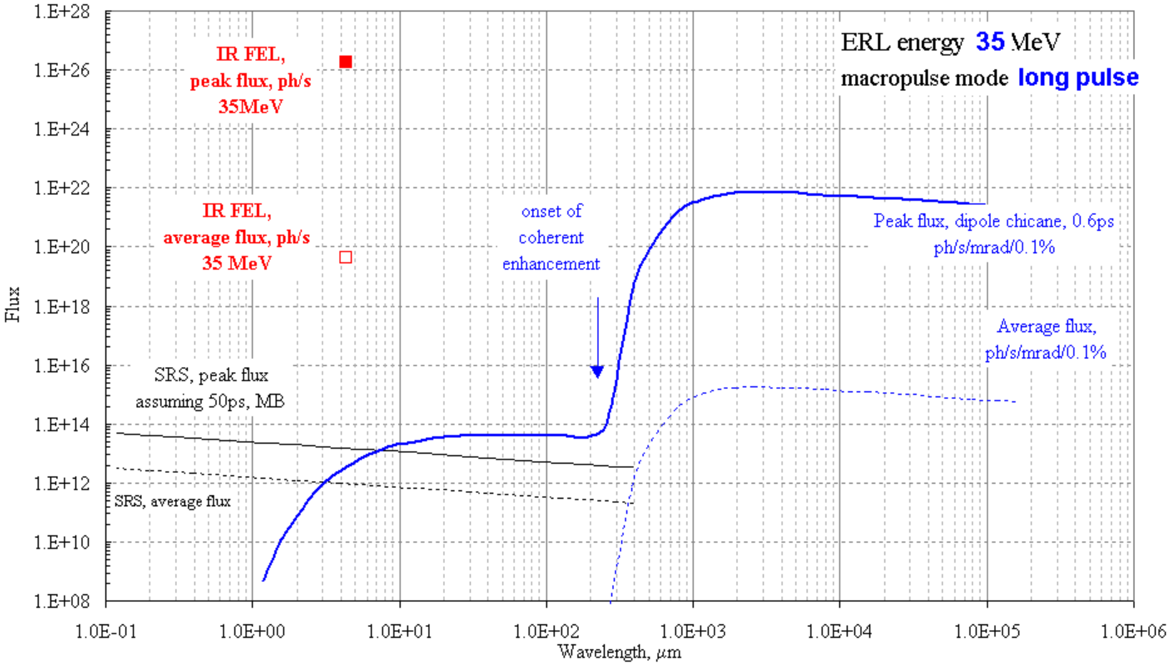

Figure 4: The calculated FEL and chicane dipole flux output characteristics of ERLP compared with those of the UK Synchrotron Radiation Source, the SRS.

4. THE 4GLS SCIENCE PROGRAMME

4GLS will enable the study of real-time molecular processes and reactions on timescales down to tens of femtoseconds in short-lived, nanostructured or ultra-dilute systems. The emphasis is on how molecules and devices ‘work’, marking a transition from the largely ‘static’ structural information obtained from 3rd generation SR. Key areas where 4GLS will make unique contributions are:

- in understanding the function of single biomolecules in living systems and membrane transport;
- determining catalytic reaction pathways (in areas as diverse as enzyme processes, reactions contributing to atmospheric pollution or occurring in the interstellar medium);
- studies of electron motion in atoms/molecules and developing ‘coherent control’ of reactions;
- developing new nanoscale devices through understanding electron charge and spin transport and
- development of new dynamic imaging techniques to improve early diagnosis of conditions such as cancer and prion-based diseases.

The major themes of the science case are time-resolved measurements and nanoscience. Particular areas of strength are high resolution pump-probe spectroscopy of atoms, molecules and clusters, including high field dynamics, dynamics at surfaces and interfaces, many body problems in condensed matter, and studies of the dynamics of biomolecules in ‘real’ environments.

The high brightness of the source will lead to step advances in research aimed at exploiting and manipulating the novel properties of systems with dimensions reduced below 10 nm. Indeed, the brightness of the source will *single* nanoscale objects to be studied, for example the distribution of electron spins in single nanoclusters of magnetic material may be determined. In some areas it will be possible to carry out an experiment in a 'single shot' or pulse of radiation; one example is photoemission using the XUV FEL combined with time-of-flight detection. The high brightness also enables the development of a number of imaging techniques, for example the use of the huge brightness of the IR-FEL to develop near-field functional imaging on truly sub-cellular (30 nm) dimensions. The high brightness of the IR and VUV FELs in combination will allow the development of imaging using sum frequency generation (SFG)[17]. Here the tunability of both sources should allow the study of a much wider range of vibrations and substrates than hitherto possible, extending its applicability to buried interfaces in systems such as metal oxide catalysts and membrane rafts. The coherent synchrotron emission seen at long wavelengths has the result that ERLs are the world's most powerful sources of THz radiation[9]. The high intensity of the bending magnet THz radiation from 4GLS will be used for experiments probing the coherent manipulation of localized semiconductor electronic states and the production and control of qubits, and for spectroscopy and imaging of biomolecules. It is anticipated that this will lead to an improved understanding of the image contrast achieved in THz medical imaging, and hence to the design of improved portable THz sources for hospitals.

The short pulse lengths provided by the source allow us to access the dynamics or kinetics of processes previously inaccessible, for example studies of real-time protein folding, molecular conformational changes and chemical reactions on timescales down to tens of fs. The flexibility and ease with which photon sources may be combined will allow unparalleled opportunities for the development of 'pump-probe' experiments. Of particular importance here are those using the VUV- and XUV-FEL sources, which allow, for example, the creation of transient, short-lived species (such as those created in the upper atmosphere or in interstellar dust clouds) and their subsequent study using continuous radiation. The variable polarization of the 4GLS sources will allow for these dynamic measurements to be used to probe free chiral molecules in the gas phase or at surfaces (for example monitorring the circular dichroism in the photoelectron angular distribution, CDAD, in free space[18,19]). This will lead to an improved understanding of the reaction pathways in asymmetric synthesis and of the origins of the homochirality of life. The brightness of the sources, particularly the XUV-FEL lead us into a new regime of high field physics where non-linear processes may be exploited[20], for example in the development of coherent photon scissors and related tools for the quantum control of chemical reactions, such as the use of phase-coherent double pulse experiments. New possibilities are opened for optical double resonance photoionization spectroscopies, using synchronised multiple photon sources. This in principle enables the study of complex molecules (such as biologically relevant species), where single photon photoelectron spectroscopy is hampered by the existence of several conformers, making interpretation of the spectra ambiguous. In two-step double resonance experiments the energy of a first photon is selected to form a well defined neutral excited state in a specific conformer. Typical lifetimes for these excited states are a few picoseconds. The prepared target thus survives long enough to be ionised by a second photon. The photoelectron can be detected and energy analysed in a time resolved manner, thereby enabling the electronic structure of a chosen conformer to be studied.

The emphasis of the 4GLS science programme is on the study of vibrational and electron dynamics using low energy spectroscopies and imaging. However, interaction of the ERL electron beam with high power laser pulses will lead to the generation of short pulsed X-rays through Thomson scattering[21]. Thus it is anticipated that a flux of hard X-rays similar to that obtained through pulse-slicing a 3rd generation SR source will be available for time-resolved diffraction and dispersive EXAFS measurements where these complement and enhance the lower energy experiments described above.

5. CONCLUSIONS

The suite of sources that is encompassed by the 4GLS facility is unprecedented in its wavelength range, flux, brightness, and flexibility of pulse structure. In addition to the major advances that will be enabled by the individual components, the synergy between the separate sources will greatly enhance their value. In particular, the ability to operate at multiple wavelengths in pump-probe configurations with a high degree of pulse-pulse synchronization will allow researchers to obtain data at sub-picosecond time resolution and with higher information content than previously possible. There are also new opportunities for developing time-resolved probeless imaging techniques to high resolution.

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